

## Numerical Modeling of Nanoelectronic Devices

Nanoelectronic Modeling 3-D (NEMO 3-D) is a computer program for numerical modeling of the electronic structure properties of a semiconductor device that is embodied in a crystal containing as many as 16 million atoms in an arbitrary configuration and that has overall dimensions of the order of tens of nanometers. The underlying mathematical model represents the quantum-mechanical behavior of the device resolved to the atomistic level of granularity. The system of electrons in the device is represented by a sparse Hamiltonian matrix that contains hundreds of millions of terms. NEMO 3-D solves the matrix equation on a Beowulf-class cluster computer, by use of a parallel-processing matrix-vector multiplication algorithm coupled to a Lanczos and/or Rayleigh-Ritz algorithm that solves for eigenvalues. In a recent update of NEMO 3-D, a new strain treatment, parameterized for bulk material properties of GaAs and InAs, was developed for two tight-binding submodels. The utility of the NEMO 3-D was demonstrated in an atomistic analysis of the effects of disorder in alloys and, in particular, in bulk  $\text{In}_x\text{Ga}_{1-x}\text{As}$  and in  $\text{In}_{0.6}\text{Ga}_{0.4}\text{As}$  quantum dots.

*This program was written by Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, and Timothy Boykin of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1).*

*This software is available for commercial licensing. Please contact Don Hart of the California Institute of Technology at (818) 393-3425. Refer to NPO-30520.*

## Organizing Diverse, Distributed Project Information

SemanticOrganizer is a software application designed to organize and integrate information generated within a distributed organization or as part of a project that involves multiple, geographically dispersed collaborators. SemanticOrganizer incorporates the capabilities of database storage, document sharing, hypermedia navigation, and semantic-interlinking into a system that can be customized to satisfy the

specific information-management needs of different user communities. The program provides a centralized repository of information that is both secure and accessible to project collaborators via the World Wide Web. SemanticOrganizer's repository can be used to collect diverse information (including forms, documents, notes, data, spreadsheets, images, and sounds) from computers at collaborators' work sites. The program organizes the information using a unique network-structured conceptual framework, wherein each node represents a data record that contains not only the original information but also metadata (in effect, standardized data that characterize the information). Links among nodes express semantic relationships among the data records. The program features a Web interface through which users enter, interlink, and/or search for information in the repository. By use of this repository, the collaborators have immediate access to the most recent project information, as well as to archived information. A key advantage to SemanticOrganizer is its ability to interlink information together in a natural fashion using customized terminology and concepts that are familiar to a user community.

*Software development activities were directed by Richard M. Keller of Ames Research Center. For further information, access <http://sciencedesk.arc.nasa.gov> and <http://io.arc.nasa.gov>.*

*Inquiries concerning rights for the commercial use of this invention should be addressed to the Patent Counsel, Ames Research Center, (650) 604-5104. Refer to ARC-15070-1.*

## Eigensolver for a Sparse, Large Hermitian Matrix

A parallel-processing computer program finds a few eigenvalues in a sparse Hermitian matrix that contains as many as 100 million diagonal elements. This program finds the eigenvalues faster, using less memory, than do other, comparable eigensolver programs. This program implements a Lanczos algorithm in the American National Standards Institute/International Organization for Standardization (ANSI/ISO) C computing language, using the Message Passing

Interface (MPI) standard to complement an eigensolver in PARPACK. [PARPACK (Parallel Arnoldi Package) is an extension, to parallel-processing computer architectures, of ARPACK (Arnoldi Package), which is a collection of Fortran 77 subroutines that solve large-scale eigenvalue problems.] The eigensolver runs on Beowulf clusters of computers at the Jet Propulsion Laboratory (JPL). The package is open-source software and is distributed under the terms of the GNU Lesser General Public License (LGPL) on the Internet through the Open Channel Foundation at <http://www.openchannelsoftware.com/>.

*This program was written by E. Robert Tisdale, Fabiano Oyafuso, Gerhard Klimeck, and R. Chris Brown of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1).*

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## Modified Polar-Format Software for Processing SAR Data

HMPF is a computer program that implements a modified polar-format algorithm for processing data from spaceborne synthetic-aperture radar (SAR) systems. Unlike prior polar-format processing algorithms, this algorithm is based on the assumption that the radar signal wavefronts are spherical rather than planar. The algorithm provides for resampling of SAR pulse data from slant range to radial distance from the center of a reference sphere that is nominally the local Earth surface. Then, invoking the projection-slice theorem, the resampled pulse data are Fourier-transformed over radial distance, arranged in the wavenumber domain according to the acquisition geometry, resampled to a Cartesian grid, and inverse-Fourier-transformed. The result of this process is the focused SAR image. HMPF, and perhaps other programs that implement variants of the algorithm, may give better accuracy than do prior algorithms for processing strip-map SAR data from high altitudes and may give better phase preservation relative to prior polar-format algorithms for processing spotlight-mode SAR data.